# Dynamic Jahn-Teller Mechanism of Superconductivity in $MgB_2$

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We propose a novel mechanism of superconductivity in $MgB_2$ based on the dynamic electronic structure of the $p\sigma$-orbitals coupled with $e_{2g}$ phonons. A nonconventional superconducting state is found to arise from electron-phonon interactions in the presence of additional pairing channels made available by the dynamic Jahn-Teller effects. A partially broken pseudo-spin symmetry in this Jahn-Teller system, together with two-phonon exchange pairing, naturally gives rise to two distinct gaps both of which are basically isotropic in the $(k_x, k_y)$ space. Important experimental observations including high $T_c$ and the anomalous specific heat are explained using this theory.

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Following the discovery of high $T_c$ superconductivity near 40 K in $MgB_2$ [1], a lot of efforts have been devoted to revealing the underlying mechanism of this novel superconductor [2]. Now it is widely agreed upon that a relatively strong electron-phonon coupling is responsible for the superconductivity of this material and there exit, at least phenomenologically, two superconducting gaps [3, 4, 5, 6, 7, 8, 9]. It has been proposed [10, 11] that the complex Fermi surfaces having both 2 dimensional (2D) cylindrical sheets and 3 dimensional (3D) tubular networks produce two gaps. However, it is still an open question whether one gap is mainly associated with the 2D cylindrical Fermi surfaces and the other is associated with the 3D Fermi surfaces.

In this letter, we propose a mechanism of superconductivity in $MgB_2$ based on a dynamic Jahn-Teller effect arising from the interplay between the doubly degenerate $p\sigma$ electronic states and the $e_{2g}$ phonon modes. The hopping motion of holes of the $p\sigma$ character on the Boron layers is constrained by the 'pseudo-spin', which will be defined later, and partial breakdown of the pseudo-spin symmetry is also important in the pairing mechanism. Unlike existing theories, we will explain both high $T_c$ and two distinct gaps in $MgB_2$ without invoking the additional 3D Fermi surface of $p\pi$ character.

According to the band structure calculations [12, 13], the $p\sigma$ states on the Boron layer form doubly degenerate $E_g$ bands at $\Gamma$ (to be precise, along the $\Gamma$A line on which the component of $\mathbf{k}$ parallel with the Boron plane, $\mathbf{k}_{||}$, is zero), where we have small hole pockets presumably responsible for the superconductivity in $MgB_2$. (Splitting of the band degeneracy away from $\Gamma$ will be taken into account later.) These hole states are known to be strongly coupled with $e_{2g}$ phonon modes with $\hbar\omega \approx 70meV$ [14, 15]. The $E_g$ hole doublet coupled with $e_{2g}$ phonon doublet states on the Boron layer can be represented by the so-called $E \otimes e$ Jahn-Teller model. A typical adiabatic potential energy surface of the $E \otimes e$ Jahn-Teller model is illustrated in Fig. 1, where $q_\theta$ and $q_\varepsilon$ correspond to the two phonon coordinates.

It is well known that one must take account of the dynamical phases of the holes and phonons in order to describe the $E \otimes e$ system properly. When the ionic configuration traverses around the potential well in Fig. 1 once, the corresponding *orbital* wavefunction of the hole (for simplicity of discussion, we leave aside the real spin wavefunction which simply follows the elementary BCS theory) acquires a phase of $-1$, as if the orbital part had spin 1/2. We call this a pseudo-spin of the hole and denote its projected value by $\alpha = \pm\frac{1}{2}$. This subject was extensively discussed in the literature [16] in the context of the Jahn-Teller effect or Berry's phase. We also note that the dynamic Jahn-Teller effect in doped $C_{60}$ superconductors was studied before, although the methods and results there were different from our work [17].

We introduce a single site Jahn-Teller Hamiltonian per unit cell using mass-weighted coordinate for the sym-

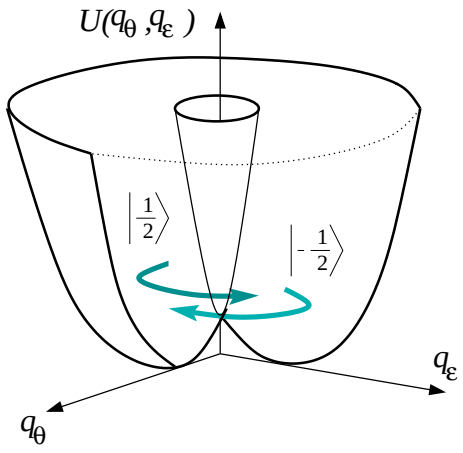


FIG. 1: Adiabatic potential surface of the $E \otimes e$ Jahn-Teller system and the doubly degenerate pseudo-spin states ($|\frac{1}{2}\rangle$, $|-\frac{1}{2}\rangle$) of the hole.

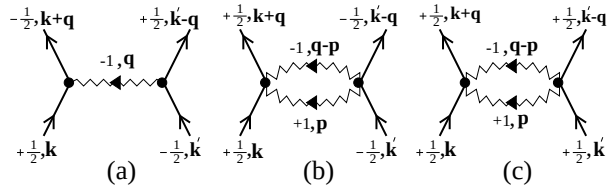


FIG. 2: Diagrams for pairing interactions with phonon exchange : (a) one-phonon exchange, and (b),(c) two-phonon exchange. The numbers indicate pseudo-spins. The obvious real spin indices are omitted for notational clarity. Diagrams with all the pseudo-spin signs switched are allowed as well (not shown).

metrized displacement $Q_\gamma(\gamma=\theta,\varepsilon)$, i.e. $q_\gamma=\sqrt{M_\gamma}Q_\gamma$,

$$h_o=\frac{1}{2}(p_\theta^2+p_\varepsilon^2)+\frac{1}{2}\omega_0^2(q_\theta^2+q_\varepsilon^2)+A(q_\theta\sigma_x+q_\varepsilon\sigma_y), \quad (1)$$

where $A$ is the hole-phonon coupling strength and $\sigma_x$, $\sigma_y$ are Pauli spin matrices for the pseudo-spin representation of $E_g$ hole doublet states. In an analogy to the 2D harmonic oscillator, the vibrational mode in the $(q_\theta, q_\varepsilon)$-space belongs to the eigenmode of the "phonon" angular momentum operator $L_z$ $(=q_\theta p_\varepsilon - q_\varepsilon p_\theta)$ with the eigenvalue of $l$, and the principal quantum number $\nu$ becomes $\nu=l+2k$ ($k$ is a non-negative integer and $-\nu\le l\le\nu$). In the present theory of superconductivity, only $\nu=0$, 1, 2 and $l=0,\pm1$ are relevant. Defining the total pseudo-spin of the system by $J_z=L_z+\frac{1}{2}\sigma_z$, it is straightforward to prove $[h_0,J_z]=0$, that is, the total pseudo-spin of the system is conserved, while individual $L_z$ and $\sigma_z$ are not. (The phonon angular momentum component, $L_z$, can be regarded as a part of the total pseudo-spin in this context.) These pseudo-spin states are derived from the $E\otimes e$ Jahn-Teller coupling between $p\sigma$ holes and $e_{2g}$ phonons, and reflect the non-adiabatic nature of the coupled states. As a consequence, relevant electron and phonon states are expected to be strongly renormalized and contribute to anomalous behaviors (e.g., broad linewidths) observed in recent photoemission spectroscopy and Raman experiments [3, 5, 18].

We generalize the theory to the Bloch state in the **k**-space of a crystal by linear combinations of the local holes of the same pseudo-spin, but mathematical details will be reserved for a longer paper [19]. We first consider the one-phonon ($\nu=1$) exchange for the Cooper pair formation. Each phonon has $l=\pm1$ in this case. In the one-phonon absorption or emission, the pseudo-spin of the hole should flip to conserve the total pseudo-spin. The only allowed one-phonon exchange mechanism is the opposite pseudo-spin Cooper pair as illustrated in Fig. 2(a). Pairing of the same pseudo-spin holes violates the conservation law in either one of the two (emission and absorption) processes. Such a selection rule has already been known in the self-energy correction to the Jahn-Teller system [20].

We next consider the two-phonon ($\nu=2$) case. In $MgB_2$, the two-phonon exchange process has been thought to be important in producing high $T_c$ and included in some previous works [10]. When we properly consider the pseudo-spin symmetry of the Jahn-Teller system such as $MgB_2$, incorporating the two-phonon exchange turns out to be essential in order to obtain two distinct gaps. Unlike the one-phonon exchange process, both opposite- and same- pseudo-spin pairs are allowed here as illustrated in Fig. 2(b) and (c). The total $l$ (sum of two individual $l$'s) of intermediate phonons is restricted to zero (i.e., the hole pseudo-spin change of $\pm2$ is not possible) to conserve the total pseudo-spin. A new model Hamiltonian with different pseudo-spin channels explicitly labelled is, in the **k**-space representation,

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1+\mathcal{H}_2+\mathcal{H}_3. \quad (2)$$

$$\mathcal{H}_0 = \sum_{\alpha\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}c^\dagger_{\alpha\mathbf{k}\sigma}c_{\alpha\mathbf{k}\sigma}, \quad (3a)$$

$$\mathcal{H}_1 = -\sum_{\alpha\mathbf{k}\mathbf{k}'}V^0_{\mathbf{k}\mathbf{k}'}c^\dagger_{-\alpha\mathbf{k}'\uparrow}c^\dagger_{\alpha-\mathbf{k}'\downarrow}c_{-\alpha-\mathbf{k}\downarrow}c_{\alpha\mathbf{k}\uparrow}, \quad (3b)$$

$$\mathcal{H}_2 = -\sum_{\alpha\mathbf{k}\mathbf{k}'}V^1_{\mathbf{k}\mathbf{k}'}c^\dagger_{\alpha\mathbf{k}'\uparrow}c^\dagger_{-\alpha-\mathbf{k}'\downarrow}c_{-\alpha-\mathbf{k}\downarrow}c_{\alpha\mathbf{k}\uparrow}, \quad (3c)$$

$$\mathcal{H}_3 = -\sum_{\alpha\mathbf{k}\mathbf{k}'}V^2_{\mathbf{k}\mathbf{k}'}c^\dagger_{\alpha\mathbf{k}'\uparrow}c^\dagger_{\alpha-\mathbf{k}'\downarrow}c_{\alpha-\mathbf{k}\downarrow}c_{\alpha\mathbf{k}\uparrow}. \quad (3d)$$

$\mathcal{H}_1$, $\mathcal{H}_2$, and $\mathcal{H}_3$ correspond to the diagrams in Fig. 2(a), (b), and (c), respectively. The explicit form of the derived interactions, $V^i_{\mathbf{k}\mathbf{k}'}$'s ($i$ =0, 1, 2), can be calculated and will be given elsewhere [19]. To discuss the nature of superconducting states, it suffices here to treat them as given parameters. The additional pairing channels due to the presence of pseudo-spin symmetry can give rise to a non-trivial superconducting ground state. Although the pairing is still based on electron-phonon interactions, the pairing order parameter can now attain more than one symmetry representation leading to the ground state with multi-dimensional order parameters while retaining the conventional $s$-wave type superconductivity.

In the pairing Hamiltonian described above, however, important features of a real crystal are missing. First, the pseudo-spin symmetry is exact only at $\mathbf{k}_{||}=0$ and there occurs small but finite deviation from the exact symmetry for $\mathbf{k}_{||}\neq0$ where Fermi surfaces actually exist. The band splitting at $\mathbf{k}_{||}\neq0$ is a clear manifestation of the breakdown of the rigorous Jahn-Teller theory for Bloch wavefunctions of $\mathbf{k}_{||}\neq0$ in a crystal as opposed to the case of a highly symmetric molecule. Second, higher-order Jahn-Teller coupling terms (not considered so far) do not commute with $J_z$ and break the pseudo-spin conservation [21]. A simple way to incorporate the symmetry breaking effect is to introduce a small symmetry breaking parameter $\phi_{\mathbf{k}}$ ($\phi_{\mathbf{k}_{||}=0}=0$ and $\phi_{\mathbf{k}_{||}\neq0}\neq0$) in the hopping Hamiltonian (Eq. (3a)) as follows,

$$\tilde{\mathcal{H}_0}=\sum_{\alpha\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}c^\dagger_{\alpha\mathbf{k}\sigma}c_{\alpha\mathbf{k}\sigma}-\sum_{\alpha\mathbf{k}\sigma}\phi_{\mathbf{k}}\varepsilon_{\mathbf{k}}c^\dagger_{\alpha\mathbf{k}\sigma}c_{-\alpha\mathbf{k}\sigma}. \quad (4)$$

This replacement naturally introduces the symmetry-breaking hopping process which gives the band splitting away from $\mathbf{k}_{||}=0$. (If the pseudo-spin $\frac{1}{2}$ were continuous symmetry ($SU(2)$) for all $\mathbf{k}$'s, there would be a single finite gap plus a zero-gap Goldstone mode, unlike the experimental observation in $MgB_2$.) Now we choose the following two order parameters, one for the opposite pseudo-spin pair and the other for the same pseudo-spin pair,

$$A_{\mathbf{k}} = \langle c_{-\frac{1}{2}-\mathbf{k}\downarrow} c_{\frac{1}{2}\mathbf{k}\uparrow}\rangle = \langle c_{\frac{1}{2}-\mathbf{k}\downarrow} c_{-\frac{1}{2}\mathbf{k}\uparrow}\rangle, \tag{5a}$$

$$B_{\mathbf{k}} = \langle c_{\frac{1}{2}-\mathbf{k}\downarrow} c_{\frac{1}{2}\mathbf{k}\uparrow}\rangle = \langle c_{-\frac{1}{2}-\mathbf{k}\downarrow} c_{-\frac{1}{2}\mathbf{k}\uparrow}\rangle. \tag{5b}$$

It is to be noted that the pseudo-spin pairing assumed above is a triplet state (even for exchange of two particles) to preserve the singlet (odd) state of the real spin pair and the s-wave (even) state of the orbital wavefunction. Following the standard mean field approximation, we can derive the effective Hamiltonian $\mathcal{H}'$ ($=\mathcal{H}-\varepsilon_F\mathcal{N}$),

$$\begin{aligned}\mathcal{H}' \simeq & \sum_{\alpha\mathbf{k}} \xi_{\mathbf{k}} (c^\dagger_{\alpha\mathbf{k}\uparrow} c_{\alpha\mathbf{k}\uparrow} - c_{-\alpha-\mathbf{k}\downarrow} c^\dagger_{-\alpha-\mathbf{k}\downarrow}) \\ & - \sum_{\alpha\mathbf{k}} \delta_{\mathbf{k}} (c^\dagger_{\alpha\mathbf{k}\uparrow} c_{-\alpha\mathbf{k}\uparrow} - c_{-\alpha-\mathbf{k}\downarrow} c^\dagger_{\alpha-\mathbf{k}\downarrow}) \\ & - \sum_{\alpha\mathbf{k}} \Delta_{1,\mathbf{k}} (c^\dagger_{\alpha\mathbf{k}\uparrow} c^\dagger_{-\alpha-\mathbf{k}\downarrow} + c_{-\alpha-\mathbf{k}\downarrow} c_{\alpha\mathbf{k}\uparrow}) \\ & - \sum_{\alpha\mathbf{k}} \Delta_{2,\mathbf{k}} (c^\dagger_{\alpha\mathbf{k}\uparrow} c^\dagger_{\alpha-\mathbf{k}\downarrow} + c_{\alpha-\mathbf{k}\downarrow} c_{\alpha\mathbf{k}\uparrow}) \\ & + (\text{constant terms}),\end{aligned} \tag{6}$$

where $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \varepsilon_F$, $\delta_{\mathbf{k}} = \phi_{\mathbf{k}}\varepsilon_{\mathbf{k}}$, and the gap-like paremeters are expressed as

$$\Delta_{1,\mathbf{k}} = \sum_{\mathbf{k}'} (V^0_{\mathbf{k}\mathbf{k}'} + V^1_{\mathbf{k}\mathbf{k}'}) A_{\mathbf{k}'}, \quad \Delta_{2,\mathbf{k}} = \sum_{\mathbf{k}'} V^2_{\mathbf{k}\mathbf{k}'} B_{\mathbf{k}'}. \tag{7}$$

Using the basis $(c^\dagger_{\frac{1}{2}\mathbf{k}\uparrow}, c^\dagger_{-\frac{1}{2}\mathbf{k}\uparrow}, c_{\frac{1}{2}-\mathbf{k}\downarrow}, c_{-\frac{1}{2}-\mathbf{k}\downarrow})$, it is convenient to cast the Hamiltonian into a matrix form (by omitting of the subscript $\mathbf{k}$ for notational simplicity),

$$\mathcal{H}' = \sum_{\mathbf{k}} \begin{pmatrix} \xi & -\delta & -\Delta_2 & -\Delta_1 \\ -\delta & \xi & -\Delta_1 & -\Delta_2 \\ -\Delta_2 & -\Delta_1 & -\xi & \delta \\ -\Delta_1 & -\Delta_2 & \delta & -\xi \end{pmatrix}. \tag{8}$$

This Hamiltonian is easily diagonalized, for each $\mathbf{k}$, yielding two positive eigenvalues,

$$E_\pm = \sqrt{(\xi \mp \delta)^2 + (\Delta_2 \pm \Delta_1)^2}. \tag{9}$$

The larger gap $\Delta_+ (= \Delta_2 + \Delta_1)$ is associated with the band of $E_{\text{normal}} = \xi - \delta$ and the smaller gap $\Delta_- (= |\Delta_2 - \Delta_1|)$ is associated with the band of $E_{\text{normal}} = \xi + \delta$. Because of this band splitting, two gaps are associated with two different normal-state (above $T_c$) densities of states (DOSs). If we define $N$ to be the normal-state DOS of unsplitted $p\sigma$ band at the Fermi level before the symmetry-breaking $\phi$ is introduced, normal-state DOSs of two bands are $N_\pm = \frac{N}{1\mp\phi}$ with the assumption of $\phi_{\mathbf{k}}$'s being independent of $\mathbf{k}$ ($\phi_{\mathbf{k}} = \phi$) in the vicinity of the Fermi level. Experimentally, it is observed that the state involved in the larger gap has the larger normal-state DOS than that of the smaller one [9]. In this situation, we naturally assign a positive value for $\phi$ ($N_+ = \frac{N}{1-\phi} > N_- = \frac{N}{1+\phi}$).

We first follow, for heuristic purposes, the approximation procedure of the weak-coupling BCS theory. We assume some *effective* cutoff energy $\omega$ and define $\lambda_1 = N(V^0 + V^1)$ and $\lambda_2 = NV^2$. Only $\lambda_1$, $\lambda_2$ and $\omega$ are independent variables for the gap equations. The coupled gap equations for finite temperature read as

$$\begin{aligned}\Delta_+ &= \frac{\lambda_2+\lambda_1}{1-\phi}\int_0^\omega d\xi \frac{\Delta_+}{2E_+}\tanh\frac{\beta E_+}{2} \\ &\quad + \frac{\lambda_2-\lambda_1}{1+\phi}\int_0^\omega d\xi \frac{\Delta_-}{2E_-}\tanh\frac{\beta E_-}{2}\ , \\ \Delta_- &= \frac{\lambda_2+\lambda_1}{1+\phi}\int_0^\omega d\xi \frac{\Delta_-}{2E_-}\tanh\frac{\beta E_-}{2} \\ &\quad + \frac{\lambda_2-\lambda_1}{1-\phi}\int_0^\omega d\xi \frac{\Delta_+}{2E_+}\tanh\frac{\beta E_+}{2}\ .\end{aligned} \tag{10}$$

By fitting to $T_c$ and the specific heat behavior, we are going to obtain below $\lambda_1 = 0.235$, $\lambda_2 = 0.25$ and $\phi = 0.2$ for the assumed value of $\hbar\omega = 74.5meV$. The normalized solutions of the above gap equations (with $\frac{\lambda_1}{\lambda_2} \simeq 0.94$ and $\phi = 0.2$) are shown in Fig. 3(a). Our theory gives two distinct gaps of the identical $T_c$ originated from two split-off $p\sigma$ bands alone, in contrast to other theories which invoke the $p\pi$ band to obtain multi-gaps. Furthermore, we predict that there exist two gaps for the same $\mathbf{k}$ vector and both gaps are basically isotropic in the Boron plane (except for a small anisotropic influence from the $p\pi$ bands located at different regions of the $\mathbf{k}$ space) unlike other theories proposing generically anisotropic gaps. Without pseudo-spins, there would be only one s-wave gap solution giving the lowest free energy. It should be possible, with angle-resolved experimental probes, to test the symmetry or angular dependence of the gap order parameters. Also, it is important in the present theory to include the symmetry-breaking parameter $\phi_{\mathbf{k}}$; otherwise, two gaps should be exactly degenerate and only one gap would manifest itself. With the same degree of approximation as in the BCS formalism, we can derive the expression for $T_c$ (weak coupling limit),

$$k_B T_c \simeq 1.13\hbar\omega \exp\left[-\frac{(\lambda_1+\lambda_2) - \sqrt{(\lambda_1-\lambda_2)^2 + 4\phi^2\lambda_1\lambda_2}}{2\lambda_1\lambda_2}\right]. \tag{11}$$

We then calculate the specific heat with this gap structure. The resulting specific heat is plotted in a usual

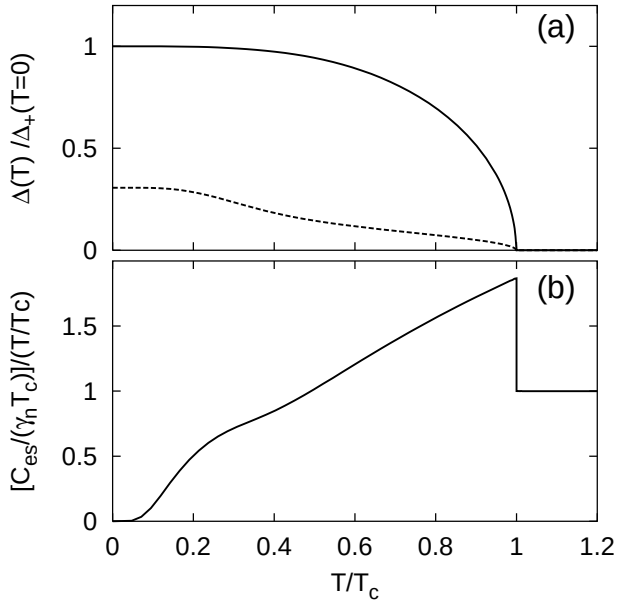


FIG. 3: (a) Solution of the self-consistent equations for two gaps $\Delta_+$ and $\Delta_-$, and (b) calculated specific heat for the above gap structure.

manner in Fig. 3(b). To obtain both $T_c = 39\ K$ and the specific heat data in agreement with experiment, we require $\phi = 0.2$, $\lambda_1 = 0.235$, $\lambda_2 = 0.25$. The symmetry breaking parameter $\phi = 0.2$ gives about the same band splitting as *ab initio* calculations for the two $p\sigma$ bands near the Fermi level. Needless to say, since $T_c$ is high and the material parameters are not in the weak-coupling limit, Eq. (11) is not to be applied directly to $MgB_2$. We have to use a more realistic (Eliashberg) equation which gives, for example, $T_c \simeq \frac{\langle\omega_{\ln}\rangle}{1.20} \exp\left[-\frac{1.04(1+\lambda)}{\lambda-(1+0.62\lambda)\mu^*}\right]$ [22]. It is beyond the scope of the present paper to calculate $\lambda_1$ and $\lambda_2$ from the first principles. The effective coupling constant $\lambda$ in the exponent in Eq. (11), namely, $\frac{2\lambda_1\lambda_2}{(\lambda_1+\lambda_2)-\sqrt{(\lambda_1-\lambda_2)^2+4\phi^2\lambda_1\lambda_2}}$ should be about 0.95, as is well known [13, 15], in order to give $T_c = 39$ K with $\mu^* = 0.13$. Then we obtain $\lambda_1 = 0.71$, $\lambda_2 = 0.76$ by simple scaling of the previous values. These values are not to be taken literally because the two-phonon exchange can modify the empirical expression for $T_c$ of the Eliashberg equation. In any cases, two-phonon exchange together with extra pairing channels makes an important contribution to $T_c$ and it is the source of larger effective $\lambda$ in $MgB_2$ than in other materials.

In summary, we have proposed a pairing mechanism in superconducting $MgB_2$ based on the dynamic Jahn-Teller effect of the doubly degenerate $p\sigma$ hole states coupled to degenerate $e_{2g}$ phonons. The pseudo-spin contraint imposed on the motion of holes by the Jahn-Teller interactions is an important factor in understanding the dynamical properties of the system. The one-phonon and two-phonon couplings lead to effective pairing interactions with additional pseudo-spin channels. As results, the high $T_c$ observed in $MgB_2$ is attributed mainly to the two-phonon exchange mechanism, and further the symmetry breaking hopping term plays a crucial role in producing two gaps which are responsible for the anomalous behaviors observed in experiment including the specific heat measurement.

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